Geomechanical/Geochemical Modeling Studies Conducted with the International Cooperative DECOVALEX-THMC Project

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RESEARCH OBJECTIVES

DECOVALEX-THMC is an international cooperative project managed by SKI, the Swedish Nuclear Power Inspectorate. The general goal is to encourage collaborative research on modeling coupled thermal-hydrological-mechanical-chemical (THMC) processes in geologic formations in support of the performance assessment for underground storage of radioactive waste. One of the ongoing research tasks within this project, initiated in 2004 by the U.S. Department of Energy (DOE), addresses the long-term impact of geomechanical and geochemical processes on flow conditions near waste emplacement drifts. The objective of this task is to (a) develop new insights into such processes and (b) to provide valuable peer-review of the respective models and their prediction results.

Table 1. Research teams and simulators applied within DOE's DECOVALEX-THMC task.

Research Team	Simulator	Coupling	Mechanical/Chemical Model	Hydraulic and Transport Model
DOE/LBNL	TOUGH-FLAC	THM	Elastic, Elastoplastic, Viscoplastic	Discrete, single or dual continuum; multiphase liquid and gas flow
DOE/LBNL	ROCMAS	THM	Elastic, Elastoplastic, Viscoplastic	Discrete or single continuum; unsaturated liquid flow; thermal vapor diffusion
BGR/Center for Applied Geosciences (Germany)	Geosys/Rockflow	THM	Elastic, Elastoplastic, Viscoplastic	Discrete or single continuum; unsaturated liquid flow; thermal vapor diffusion
CAS, Chinese Academy of Sciences	FRT-THM	THM	Elastic, Elastoplastic, Viscoplastic	Discrete or single continuum; unsaturated liquid flow; thermal vapor diffusion
JAEA, Japan Atomic Energy Agency	THAMES	THM	Elastic, Elastoplastic, Viscoplastic	Discrete or single continuum; unsaturated liquid flow; thermal vapor diffusion
DOE/LBNL	TOUGHREACT	THC	Equilibrium and kinetic mineral-water-gas reactions HKF activity model	Discrete, single or dual continuum; multiphase liquid and gas flow; advection/ diffusion of total concentrations (sequential)
BGR/Center for Applied Geosciences (Germany)	Geosys/Rockflow with PHREEQC	THC	PHREEQC	Discrete or single continuum; unsaturated liquid flow; thermal vapor diffusion; advection/diffusion of total concentrations (sequential)
JAEA, Japan Atomic Energy Agency	THAMES with Dtransu-3D-EL and PHREEQC	THMC	PHREEQC	Discrete or single continuum; unsaturated liquid flow; thermal vapor diffusion; advection/ diffusion of total concentrations (sequential)

APPROACH

The four research teams (from China, Germany, Japan, and USA) participating in DOE's task within the DECOVALEX-THMC project were asked to conduct predictive analysis of the long-term coupled processes in generic repositories with simplified conditions and geometry. Participating research teams model the THMC processes in the fractured rock close to a representative emplacement drift as a function of time, predict long-term changes in hydrological properties, and evaluate the impact on near-field flow and transport processes. Two generic repositories situated in different host rock types and featuring different emplacement conditions are analyzed for comparison. One is a simplified repository model of the United States' Yucca Mountain site, a deep unsaturated volcanic rock formation with emplacement in open gas-filled drifts. The second repository model is "located" in saturated crystalline rock, with emplacement drifts backfilled using a low-permeability buffer material such as bentonite (a concept considered in many European countries and in Japan).

ACCOMPLISHMENTS

As shown in Table 1, the research teams use different codes with different model approaches and characteristics. Since all teams simulate the same task configuration, research results from the participating teams can be directly compared. To date, good progress has been made in both model development and application. Comparison of geomechanical results indicates good overall agreement with respect to temperatures, stresses, and various hydrological parameters, despite the fact that different model approaches were used. Geochemical models show good quantitative agreement regarding aqueous species concentrations, while some differences with respect to mineral alterations still need to be worked out.

SIGNIFICANCE OF FINDINGS

The collaborative research conducted by international teams helps to develop a broader understanding of the complex THMC processes occurring near geologic repositories for radioactive waste. Good agreement between simulation results obtained with different model approaches provides enhanced confidence in their predictive capabilities when applied, for example, to the proposed Yucca Mountain repository.

RELATED PUBLICATIONS

Birkholzer, J., D. Barr, J. Rutqvist, and E.L. Sonnenthal, Motivation, description, and summary status of geomechanical and geochemical modeling studies in Task D of the International DECOVALEX Project. Proceedings, Geoproc 2006, China, May 2006.

Rutqvist, J., J. Birkholzer, M. Chijimatsu, O. Kolditz, Q. Liu, Y. Oda, W. Wang, and C. Zhang, Comparative simulation study on coupled THM processes near back-filled and open-drift nuclear waste repositories in Task D of the International DECOVALEX Project. Proceedings Geoproc 2006, China, May 2006.

Xie, M., E.L. Sonnenthal, W. Wang, O. Kolditz, J. Birkholzer, Y. Oda, and M. Chijimatsu, Geochemical predictions for a hypothetic repository located in saturated crystalline rock—Comparative evaluation of two different research teams. Proceedings Geoproc 2006, China, May 2006.

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